

Hybridization oscillation in the one-dimensional Kondo-Heisenberg model with Kondo holes

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We use the density matrix renormalization group method to study the properties of the one-dimensional Kondo-Heisenberg model doped with Kondo holes. We find that the perturbation of the Kondo holes to the local hybridization exhibits spatial oscillation pattern and its amplitude decays exponentially with distance away from the Kondo hole sites. The hybridization oscillation is correlated with both the charge density oscillation of the conduction electrons and the oscillation in the correlation function of the Heisenberg spins. In particular, we find that the oscillation wavelength for intermediate Kondo couplings is given by the Fermi wavevector of the large Fermi surface even before it is formed. This suggests that heavy electrons responsible for the oscillation are already present in this regime and start to accumulate around the to-be-formed large Fermi surface in the Brillouin zone. Our results suggest a new way to probe the heavy electron emergence by using the scanning tunneling spectroscopy.

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Heavy fermion materials exhibit many exotic quantum phenomena such as unconventional superconductivity [1–3] and unconventional quantum criticality [4–6]. The existence of these exotic quantum states is closely related to the host state, namely the heavy electron Kondo liquid, which emerges below a characteristic temperature, T^* , due to the collective hybridization of a lattice of localized f -spins with the conduction electron sea [7, 8]. While the so-called Kondo problem of a single localized moment antiferromagnetically coupled to the conduction electrons has been well understood, the Kondo lattice problem remains controversial and poses a long standing challenge for the condensed matter community [9–11]. The difficulty lies in the lack of a good understanding of the collective nature of the underlying spin entanglement or hybridization between the localized spins and the conduction electrons [12]. Recently, it was realized that by introducing local Kondo holes, or defects/nonmagnetic impurities in the lattice of the local moments [13–15], it is possible to stimulate a collective spatial modulation in the hybridization strength which can be probed by using the state-of-the-art spectroscopic imaging scanning tunneling microscopy (STM) [16, 17]. Theoretical calculations based on the mean-field approximation predicted a spatial oscillation of the hybridization with a characteristic wavelength determined by the Fermi wavevector of the so-called small Fermi surface of unhybridized conduction electrons [13], which seems to be confirmed by later STM experiment on Th-doped URu₂Si₂ at very low temperature in the hidden order phase [16].

Bearing in mind the limitation of the mean-field approximation, we examine the above results by applying the density matrix renormalization group (DMRG)

method [18–20] to the one-dimensional (1D) Kondo-Heisenberg model doped with Kondo holes. This allows us to solve the model exactly and take into fully account magnetic quantum fluctuations that are beyond the mean-field approximation [7, 8]. Our results confirm the predicted hybridization oscillation induced by the Kondo holes. However, contrary to the mean-field prediction, the characteristic wavelength of the oscillation changes dramatically from weak coupling to strong coupling regimes. For both intermediate and strong couplings, we find that the local hybridization, the conduction electron charge density, and the correlation function of the Heisenberg spins are all entangled and exhibit similar oscillation pattern. In particular, away from half filling, we find that the oscillation wavelength is determined by the Fermi wavevector of the large Fermi surface even before it is formed, distinctly different from previous mean-field predictions for the charge density oscillation. This indicates that preformed heavy electrons are already present and start to accumulate around the to-be-formed large Fermi surface at intermediate couplings.

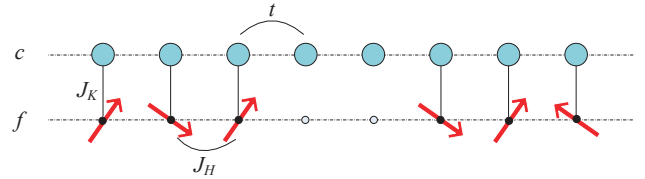


FIG. 1: (color online) An illustration of the one-dimensional Kondo-Heisenberg model with Kondo holes in the middle of the spin chain.

Our results suggest that these emergent heavy electrons can be detected by the Kondo hole induced hybridization oscillation using the scanning tunneling spectroscopy.

We start with the following Hamiltonian for the 1D Kondo-Heisenberg model with Kondo holes,

$$H = -t \sum_{i,\sigma} \left(c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.} \right) + J_K \sum_i ' \vec{S}_i \cdot \vec{s}_i + J_H \sum_i ' \vec{S}_i \cdot \vec{S}_{i+1}, \quad (1)$$

where the sum (\sum') is over all spin sites other than the hole sites located in the middle of the Heisenberg chain as illustrated in Fig. 1. $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) is the creation (annihilation) operator of the conduction electron with spin σ at the i -th site ($i = 1, \dots, L$) and $\vec{s}_i = \sum_{\sigma,\sigma'} c_{i,\sigma}^\dagger (\vec{\sigma}/2)_{\sigma,\sigma'} c_{i,\sigma'}$, where $\vec{\sigma}$ are the Pauli matrices, defines the spin density operator. \vec{S}_i denotes the local Heisenberg spin at the i -th site. t is the hopping parameter of the conduction electrons between neighboring sites, and $J_K/t > 0$ is the local Kondo coupling. We further introduce a finite antiferromagnetic exchange coupling $J_H/t = 0.5$ between nearest-neighbor Heisenberg spins to avoid possible ferromagnetic ground state away from half filling [21–24]. For numerical simplicity, we remove two local spins ($i_h = L/2, L/2 + 1$) to keep the inversion symmetry and a nonmagnetic ground state. The results are similar but less pronounced if only one local spin is removed. The model is calculated with a modified DMRG++ code [25] using 800 block states for $L = 100$ sites and with open boundary condition. The presented results have been verified to converge with different numbers of lattice sites and block states and also examined using the exact diagonalization method on a lattice of up to 14 sites with both periodic and open boundary conditions. Similar conclusions are also obtained in a ladder system with $L = 50$. We consider the ground state $S_{tot}^z = \sum_i s_i^z + \sum_i ' S_i^z = 0$ for each fixed average occupation number of the conduction electrons, $n^c = L^{-1} \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}$. To avoid the boundary effect [26, 27], we subtract the results of the corresponding clean Kondo lattice without the Kondo holes and study the changes in the local hybridization, $\delta\mathcal{V}_i = \langle \vec{S}_i \cdot \vec{s}_i \rangle - \langle \vec{S}_i \cdot \vec{s}_i \rangle_0$, the charge density of the conduction electrons, $\delta n_i^c = \sum_{\sigma} \left(\langle c_{i,\sigma}^\dagger c_{i,\sigma} \rangle - \langle c_{i,\sigma}^\dagger c_{i,\sigma} \rangle_0 \right)$, and the correlation function of local spins, $\delta\chi_i = \langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle - \langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle_0$. The subscript "0" indicates the corresponding results for the clean Kondo lattice as a background for comparison.

We first discuss the results for $n^c < 1$, namely away from the half filling. Fig. 2 presents some typical results with $n^c = 0.2$ and 0.8 for different Kondo couplings, J_K/t . As expected, the resulting $\delta n_i^c < 0$ at the Kondo hole sites is distinctly different from that induced by an attractive nonmagnetic impurity. We observe spatial oscillations in almost all the cases and the amplitude of

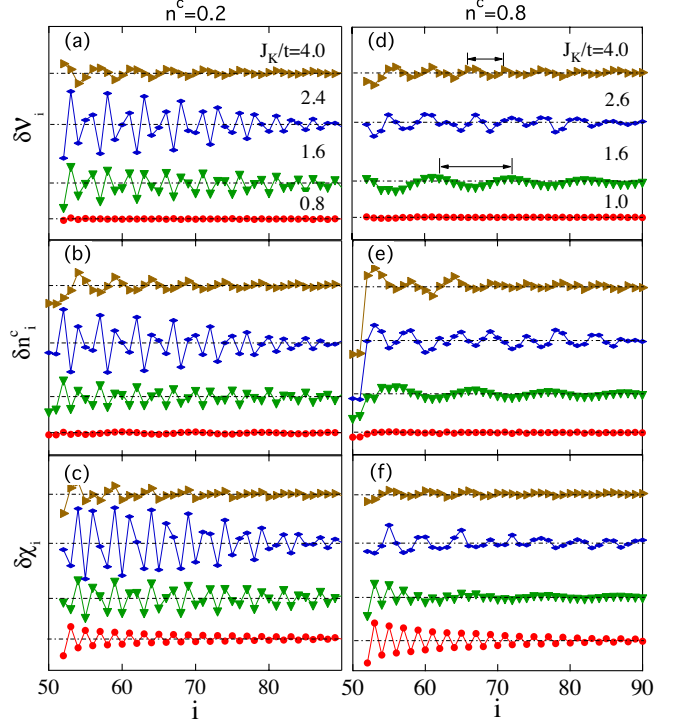


FIG. 2: (color online) The variation of the spatial oscillation patterns induced by the Kondo holes for $\delta\mathcal{V}_i$, δn_i^c and $\delta\chi_i$ with the Kondo coupling J_K/t . Other parameters are $J_H/t = 0.5$ and $L = 100$ for both $n^c = 0.2$ and 0.8 .

the oscillation decays gradually with distance away from the hole sites. A straightforward comparison of the results at different J_K/t indicates that the wavelength of the oscillation changes dramatically from the weak coupling regime to the strong coupling regime. Moreover, there seems to be a close correlation of the oscillation wavelength in all three quantities in the strong coupling regime. In the weak coupling regime, on the other hand, the oscillation is hardly seen in $\delta\mathcal{V}_i$, whereas the charge density δn_i^c and the spin correlation, $\delta\chi_i$, also exhibit different oscillation patterns, suggesting that the conduction electrons are not strongly coupled with the local spins.

To see these results more clearly, we present in Fig. 3 the Fourier transforms of $\delta\mathcal{V}_i$, δn_i^c , and $\delta\chi_i$ in the momentum space for $n^c = 0.2$, where the features are more pronounced. We see that all spectra exhibit peak structures. For $J_K/t = 0.8$ in the weak coupling regime, $\delta\mathcal{V}(k)$ is negligible small with only a tiny peak at $k = \pi$. In contrast, $\delta\chi(k)$ shows a sharp peak at $k = \pi$ due to the strong inter-site antiferromagnetic correlations between neighboring spins, and $\delta n^c(k)$ has two peaks at $k = \pi n^c = 2k_F^c$ and $k = \pi$ where the former corresponds to the small Fermi surface of the conduction electrons and the latter comes from the influence of the spin chain as

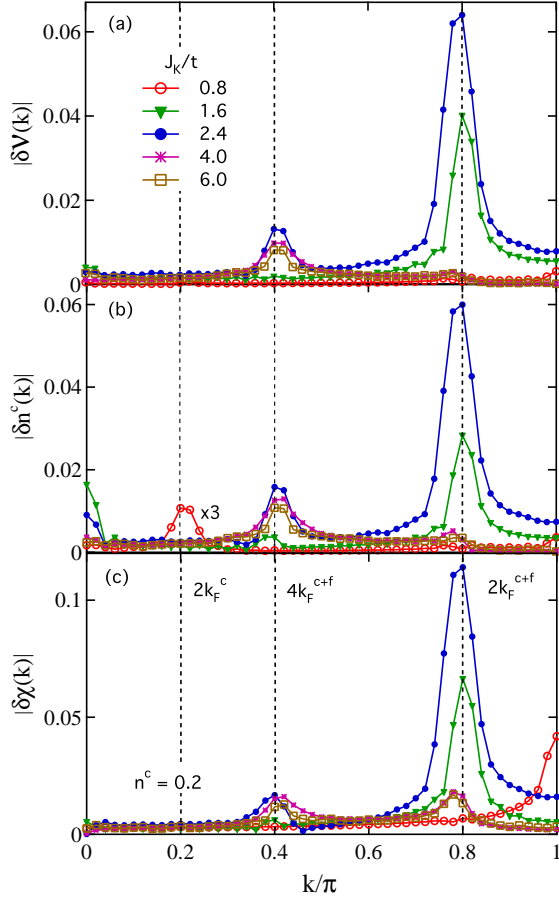


FIG. 3: (color online) Absolute values of the Fourier transforms of $\delta\mathcal{V}_i$, δn_i^c and $\delta\chi_i$ for $n^c = 0.2$, $J_H/t = 0.5$ and different Kondo couplings, J_K/t .

is the case for the small peak at $k = \pi$ in $\delta\mathcal{V}_i$. The weak oscillations in both $\delta\mathcal{V}_i$ and $\delta\chi_i$ indicate that the conduction electrons and the local spins are effectively decoupled (or only very weakly coupled). For $J_K/t = 1.6$ in the intermediate coupling regime, a sharp peak appears at $k = \pi(1 - n^c) = 2k_F^{c+f} \pmod{2\pi}$ in all three quantities. Here k_F^{c+f} is the Fermi wavevector of the large Fermi surface, indicating that the conduction electrons are now coupled to the local spins and the large Fermi surface starts to take effect. For $J_K/t = 2.4$, a new peak emerges at $k = 2\pi n^c$, which corresponds to either $4k_F^c$ or $4k_F^{c+f} \pmod{2\pi}$. Further increasing J_K/t seems to suppress the peak at $2k_F^{c+f}$ but keep the peak at $4k_F^{c+f}$ almost unchanged. We note that the $4k_F^{c+f}$ or $4k_F^c$ oscillation may be understood as a special one-dimensional feature that originates from the spinless hole Fermi surface due to complete spin-charge separation following the formation of the Kondo singlets between the conduction electrons and the local spins [26]. Although we cannot distinguish $4k_F^c$ from $4k_F^{c+f} \pmod{2\pi}$ by number, we at-

tempt to ascribe this peak to $4k_F^{c+f} \pmod{2\pi}$ associated with the large Fermi surface because of its coexistence with the $2k_F^{c+f}$ peak, whereas the $2k_F^c$ peak is absent in these regimes.

We note that the critical Kondo coupling is about $J_K/t \approx 3.0$ for $n^c = 0.2$ and $J_H/t = 0.5$ in the clean Kondo lattice [24]. It is quite unexpected that the hybridization oscillation is determined by k_F^{c+f} at $J_K/t = 1.6$ and 2.4 before the large Fermi surface is even formed. This implies that heavy electrons are already present in this intermediate coupling regime and start to accumulate around k_F^{c+f} in the momentum space. Our results for $n^c < 1$ suggest three regimes of the Kondo lattice physics depending on the magnitude of J_K/t : (1) the weak coupling regime where the conduction electrons and the local spins are effectively decoupled (or only very weakly coupled); (2) the strong coupling regime where the two components are coupled to give rise to a well-defined large Fermi surface and complete spin-charge separation in 1D (corresponding to the $4k_F^{c+f}$ peak); (3) the intermediate regime where the large Fermi surface is not yet formed, but preformed heavy electrons are already present and all three quantities, $\delta\mathcal{V}_i$, δn_i^c and $\delta\chi_i$, exhibit similar oscillation pattern (corresponding to the $2k_F^{c+f}$ peak). These preformed heavy electrons are primarily responsible for the charge density and hybridization oscillations induced by the Kondo holes, whereas local spin singlets are not fully established so that the hybridization must be collective in nature and the global spin singlet state must involve highly nonlocal entanglement between neighboring spins and conduction electrons.

We point out that previous mean-field calculations predicted different periodicity for the three quantities, with $2k_F^c$ for δn_i^c and $\delta\mathcal{V}_i$ and $2k_F^{c+f}$ for $\delta\chi_i$ in all parameter regimes [13]. This is in contradiction with our results where all three quantities have the same periodicity in the intermediate and strong coupling regimes. At the moment it is not clear what causes this discrepancy. It could be due to the one dimensional nature (with strong quantum fluctuations) of our DMRG calculations. However, our calculations on a ladder ($L = 50$) yield similar oscillation patterns. Also, it is natural to imagine that all three quantities should be strongly entangled and have the same periodicity at least in the strong coupling regime. Moreover, the same $2k_F^{c+f}$ oscillation for the spin correlation $\delta\chi_i$ obtained in our approach and the mean-field approach seems to support the idea that our results may still be valid in higher dimensions. If this is the case, one may attempt to think that the mean-field calculations yield wrong predictions for treating incorrectly (as simple hybridization bands) the correlated states of collectively entangled conduction electrons and local spins. A thorough investigation of this discrepancy may lead to a deeper understanding of the various approaches to the Kondo lattice problem. Careful analysis and numer-

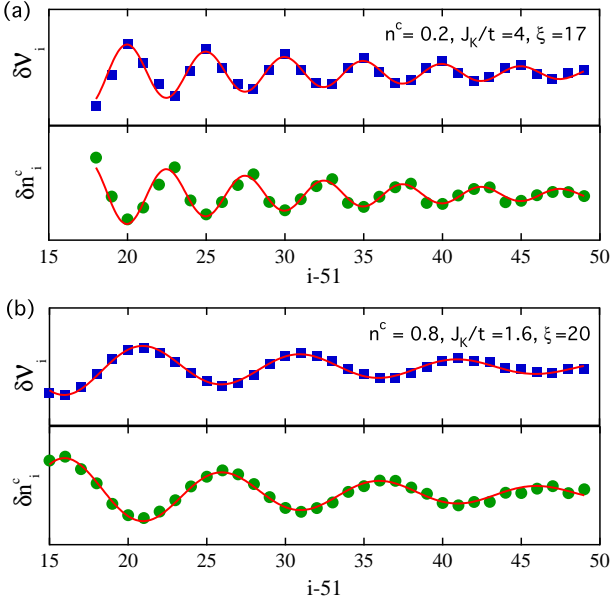


FIG. 4: (color online) Fit to $\delta\mathcal{V}_i$ and δn_i^c for (a) $n^c = 0.2$ and $J_K/t = 4$; (b) $n^c = 0.8$ and $J_K/t = 1.6$. The solid lines are the fitting curves.

ical calculations in higher dimensions will be crucial in order to clarify the role of quantum fluctuations in determining the oscillation pattern. As a consequence, the observation of the hybridization oscillation at the small Fermi wavevector in the hidden order phase of Th-doped URu₂Si₂ may probably need to be reinterpreted or reexamined in the normal state [16].

To obtain a quantitative understanding of the spatial decay of the oscillation, we consider two examples where the spectra are governed by one dominant sharp peak in the momentum space. The correlation functions are then fitted using the following form in real space,

$$\begin{aligned}\delta\mathcal{V}_i &= A_V \cos(2\pi x_i/\lambda + \theta_V) e^{-x_i/\xi_V}, \\ \delta n_i^c &= A_n \cos(2\pi x_i/\lambda + \theta_n) e^{-x_i/\xi_n},\end{aligned}\quad (2)$$

where the oscillation wavelength λ is the same for the two quantities as discussed above and $x_i = i - L/2 - 1$ is the distance of the i -th lattice site from the Kondo holes. $\theta_{V/n}$ is the phase shift and $\xi_{V/n}$ denotes the characteristic decay length of the oscillation. Fig. 4 shows two examples at $n^c = 0.2$ and 0.8 . We find an excellent agreement for both $\delta\mathcal{V}_i$ and δn_i^c . Both quantities exhibit similar decay lengths, $\xi_V = \xi_n = \xi$. On the other hand, the oscillation in $\delta\chi_i$ in the strong coupling regime has a smaller decay length, despite that it exhibits the same periodicity. This suggests that the oscillation in $\delta\mathcal{V}_i$ is most affected by the charge density oscillation for $n^c < 1$. We note that the above data do not follow a power law decay that is typically expected for the correlation function in 1D systems. This may be easily understood since we are

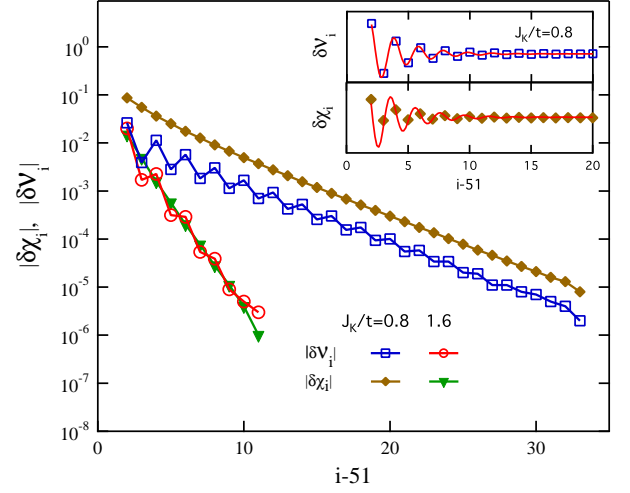


FIG. 5: (color online) A semilog plot for the absolute values of $\delta\mathcal{V}_i$ and $\delta\chi_i$ as a function of the distance from the Kondo holes for $n^c = 1$ and $J_K/t = 0.8, 1.6$. The inset shows the original data, $\delta\mathcal{V}_i$ and $\delta\chi_i$, for $J_K/t = 0.8$ on the linear scale.

dealing with perturbation in "local" quantities instead of spatial correlations at long distances.

Next we study briefly the half-filling case at $n^c = 1$, where the density oscillation is suppressed due to the particle-hole symmetry and the finite charge gap. We therefore only need to consider the local hybridization $\delta\mathcal{V}_i$ and the spin correlation function $\delta\chi_i$. Fig. 5 compares the two quantities on a logarithmic-linear scale as a function of the distance from the Kondo holes. We see that $|\delta\mathcal{V}_i|$ and $|\delta\chi_i|$ exhibit similar slope ($\propto \xi_V^{-1}$) with distance and similar oscillation pattern originating from the antiferromagnetic correlations in the spin chain (see the inset in Fig. 5). The good linearity confirms clearly the exponential decay of the oscillation amplitude and provides a further support for our analysis for $n^c < 1$. We obtain $\xi_V = 3$ for $J_K/t = 0.8$ and $\xi_V = 1$ for $J_K/t = 1.6$. No oscillation is observed for larger J_K/t . This indicates that $J_K/t = 1.6$ locates at the boundary of weak and intermediate couplings for $n_c = 1$. The very rapid suppression of the oscillation at $n^c = 1$ suggests that the charge oscillation (for $n^c < 1$) plays the role of an enhancer for the hybridization oscillation. The absence of spatial oscillation for larger J_K/t is consistent with our observed $2k_F^{c+f} \pmod{2\pi}$ periodicity for $n^c < 1$, but contradicts the mean-field calculations which predicted a wavevector $k = 2k_F^c = \pi n^c$ in the hybridization oscillation [13]. This difference may provide a possible clue for understanding the discrepancy. In our calculations, the absence of the spatial oscillation for larger J_K/t may be attributed to the effective localization of the redundant conduction electron at the impurity site caused by the large hybridization gap created by the Kondo coupling at its undoped nearest-neighbor sites. The crossover from

weak to intermediate couplings reflects the competition between the kinetic energy and the hybridization energy. It would be interesting to check if this charge localization is present in the mean-field calculations.

To summarize, we use the density matrix renormalization group method to study the perturbation in the local hybridization, the charge density of the conduction electrons and the correlation function of the local spins induced by Kondo holes in the 1D Kondo-Heisenberg model. We find that all three quantities exhibit spatial oscillations whose amplitude decay exponentially with distance away from the Kondo holes. Our results indicate that the hybridization oscillation is closely related to the oscillations in the conduction electron charge density and the antiferromagnetic spin correlations. At half filling, where the charge density oscillation is suppressed, the antiferromagnetic spin correlations play the major role in determining the hybridization oscillation. Away from half filling, the charge density oscillation plays the dominant role and determines the wavelength and the decay length of the hybridization oscillation. We find three different regimes in the oscillation pattern. In the intermediate and strong coupling regimes, the wavelength is given by the Fermi wavevector of the large Fermi surface, implying the presence of heavy electrons around the large Fermi surface even before it is well formed. Our results suggest a new way to detect the heavy electron emergence using the scanning tunneling spectroscopy. Moreover, the derived large decay length indicates that the Kondo lattice physics is highly nonlocal. This excludes any attempt based on local approximations and demands a proper treatment of the nonlocal and collective nature of the lattice hybridization in pursuit of a satisfactory solution to the Kondo lattice problem.

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- [1] F. Steglich, J. Aarts, C. D. Bredl, W. Lieke, D. Meschede, W. Franz, and H. Schäfer, *Phys. Rev. Lett.* **43**, 1892 (1979).
- [2] C. Pfleiderer, *Rev. Mod. Phys.* **81**, 1551 (2009).
- [3] B. D. White, J. D. Thompson, and M. B. Maple, *Physica C* **514**, 246 (2015).
- [4] P. Coleman, C. Pépin, Q. Si, and R. Ramazashvili, *J. Phys.: Condens. Matt.* **13**, 723 (2001).
- [5] Q. Si, S. Rabello, K. Ingersent and J. L. Smith, *Nature (London)* **413**, 804 (2001).
- [6] O. Stockert and F. Steglich, *Annu. Rev. Condens. Matt. Phys.* **2**, 79 (2011).
- [7] Y.-F. Yang, Z. Fisk, H.-O. Lee, J. D. Thompson, and D. Pines, *Nature (London)* **454**, 611 (2008).
- [8] Y.-F. Yang and D. Pines, *Proc. Natl. Acad. Sci. USA* **109**, E3060 (2012).
- [9] A. C. Hewson, *The Kondo Problem to Heavy Fermions*, (Cambridge Univ. Press, 1993).
- [10] P. Coleman, in *Handbook of Magnetism and Advanced Magnetic Materials*, edited by H. Kronmüller and S. Parkin (Wiley and Sons, New York, 2007).
- [11] Y.-F. Yang, *Rep. Prog. Phys.* **79**, 074501 (2016).
- [12] G. Lonzarich, D. Pines, and Y.-F. Yang, *arXiv:1601.06050* (2016).
- [13] J. Figgins and D. K. Morr, *Phys. Rev. Lett.* **107**, 066401 (2011).
- [14] J. X. Zhu, J. -P. Julien, Y. Dubi, and A. V. Balatsky, *Phys. Rev. Lett.* **108**, 186401 (2012).
- [15] P. P. Baruselli and M. Vojta, *Phys. Rev. B* **89**, 205105 (2014).
- [16] M. H. Hamidian, A. R. Schmidt, I. A. Firmo, M. P. Allan, P. Bradley, J. D. Garrett, T. J. Williams, G. M. Luke, Y. Dubi, A. V. Balatsky, and J. C. Davis, *Proc. Natl. Acad. Sci. USA* **108**, 18233 (2011).
- [17] A. Yazdani, E. H. da Silva Neto, and P. Aynajian, *Annu. Rev. Condens. Matt. Phys.* **7**, 11 (2016).
- [18] S. R. White, *Phys. Rev. Lett.* **69**, 2863 (1992).
- [19] S. R. White, *Phys. Rev. B* **48**, 10345 (1993).
- [20] U. Schollwöck, *Rev. Mod. Phys.* **77**, 259 (2005).
- [21] H. Tsunetsugu, M. Sigrist, and K. Ueda, *Rev. Mod. Phys.* **69**, 809 (1997).
- [22] M. Gulàcsi, *Adv. Phys.* **53**, 769 (2004).
- [23] S. Moukouri and L. G. Caron, *Phys. Rev. B* **54**, 12212 (1996).
- [24] N. Xie and Y.-F. Yang, *Phys. Rev. B* **91**, 195116 (2015).
- [25] G. Alvarez, *Comput. Phys. Commun.* **180**, 1572 (2009).
- [26] N. Shibata, K. Ueda, T. Nishino, and C. Ishii, *Phys. Rev. B* **54**, 13495 (1996).
- [27] J. C. Xavier, E. Novais, and E. Miranda, *Phys. Rev. B* **65**, 214406 (2002).

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